LA-UR-22-20929

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Title: Improved Time-Stepping Methods in Global to Regional Ocean Modeling
Annual Status Report, 2021 LANL Institutional Computing

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Intended for: Report

Issued: 2022-02-03

Los Alamos
NATIONAL LABORATORY

Improved Time-Stepping Methods in Global to Regional Ocean Modeling

Annual Status Report, 2021
LANL Institutional Computing account w20_ocean_time_step
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LA-UR-22-XXXX

Scientific and Programmatic Impact

Time stepping algorithms are an important part of ocean models, and strongly influence both the accuracy of solution and performance. There have been a number of projects investigating various improvements for ocean time-stepping schemes in the Model for Prediction Across Scales-Ocean (MPAS-Ocean), a component of the DOE Energy Exascale Earth System Model.

Ocean dynamics include fast surface gravity waves, which are two-dimensional, and slower internal waves, which are three-dimensional, so ocean models use a split time-stepping scheme that separates these barotropic and baroclinic modes for efficiency. MPAS-Ocean runs on variable-resolution horizontal meshes, and must scale to tens of thousands of cores and millions of horizontal gridcells. Ocean models require time stepping algorithms that are customized to these needs, and which are tuned for performance on various resolutions and architectures.

Here we summarize each project using LANL Institutional Computing resources, account w20_ocean_time_step.

Local Time Stepping
Giacomo Capodaglio, post-doc, now staff, Mark Petersen, advisor, Jeremy Lilly, student
Local time stepping was implemented in the MPAS shallow water core and published in Capodaglio and Petersen (2022). Dr. Capodaglio then implemented LTS in the MPAS-Ocean core, which is currently being tested by LANL student Jeremy Lilly, a PhD student from Oregon State, in a test case for coastal inundation for Delaware Bay. LTS was the topic of Jeremy's summer research internship while at LANL in 2021.

Summary: To numerically solve equations on variable-resolution grids with regions of high spatial resolution, global time-stepping schemes employ the same small time step across the entire domain. This slows down the simulation. Researchers carried out an efficient parallel implementation and performance assessment of LTS schemes for the shallow water equations in MPAS, which is also used for ocean and climate simulations. These methods are fast, accurate, and scalable in a high-performance computing setting. Moreover, the scheme with convergence order three showed a reduction in terms of computational time of up to 70 percent compared to a Runge-Kutta scheme of order four on certain variable-resolution meshes.

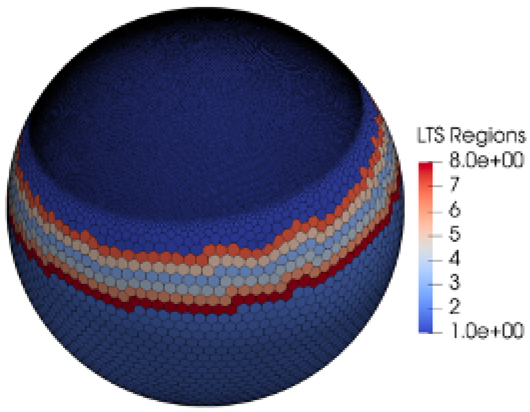

Figure 1. Representation of the different regions employed for the time-stepping procedure. Some of the intermediate layers represent interface regions that allow communication between the coarse and fine time-step regions.

A Suite of Verification Exercises for Barotropic Solver of Ocean Models
Siddhartha Bishnu, graduate student (LANL, Fl. State), now LANL post-doctoral researcher, Mark Petersen
Sid successfully defended his thesis in June 2021, using research with simulations run on LANL IC.

Part I: On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs:
Here we discuss the leading order terms of the local truncation error of hyperbolic partial differential equations (PDEs). If one employs a stable numerical scheme and the global solution error is of the same order of accuracy as the global truncation error, one can make the following observations in the asymptotic regime, where the truncation error is dominated by the powers of grid-spacing and time step rather than their coefficients. Assuming that the spatial and temporal resolutions reach the asymptotic regime before the machine precision error dominates,
i. the order of convergence of stable numerical solutions of hyperbolic PDEs at constant ratio of time step to grid-spacing is governed by the minimum of the orders of the spatial and temporal discretizations, and
ii. convergence cannot even be guaranteed under only spatial or temporal refinement.
I have tested the theory against numerical methods employing Method of Lines and not against ones that treat space and time together. Otherwise, the theory applies to any hyperbolic PDE, be it linear or non-linear, and employing finite difference, finite volume, or finite element discretization in space, and advanced in time with a predictor-corrector, multistep, or a deferred correction method. If the PDE is reduced to an ordinary differential equation (ODE) by specifying all spatial gradients to be zero, then the standard local truncation error of the ODE is recovered. I perform the analysis with

generic and specific hyperbolic PDEs using the symbolic algebra package SymPy, and conduct a number of numerical experiments to demonstrate the theoretical findings.

Part II: Time-Stepping Methods for Ocean Models: In the second part of my doctoral research, I study and address some complications associated with time-stepping the prognostic equations of an ocean model. The primary one is the disparate time scales problem, leading to a splitting of the fast depth-independent 2D barotropic modes and the slow 3D baroclinic modes, and the application of a time-averaging filter over the barotropic modes to minimize aliasing and mode-splitting errors. To study the combined stabilizing effect of various filters and the forward-backward parameter, I develop a non-linear shallow water solver, simulate a surface gravity wave, and use the magnitude of the SSH error norm as an indicator of the right amount of dissipation. I redesign parts of the time-stepping algorithm of the Model for Prediction Across Scales — Ocean (MPAS-O) developed at the Los Alamos National Laboratory (LANL), to improve the barotropic-baroclinic splitting and enhance the coupling between the two modes. I incorporate a number of barotropic time-averaging filters in MPAS-O. I repeat the surface gravity wave test case with the non-rotating primitive equations of MPAS-O, and analyze the influence of the filters on the numerical solution. Finally, I design a verification suite of shallow water test cases for the barotropic solver of ocean models. I develop an unstructured-mesh ocean model in object- oriented Python, employing the TRiSK-based spatial discretization of MPAS-O, and numerous time- stepping methods, and use it as the platform to run the shallow water test cases. I conclude my doctoral research by conducting convergence studies for each test case keeping the time step proportional to cell width, and verifying that the convergence rates match the ones predicted by the theory in part (a).

A modified TRiSK scheme to address instabilities found in MPAS-Ocean
Sara Calandrini, post-doc, Mark Petersen, Darren Engwirda
In MPAS-O the horizontal discretization used is the TRiSK scheme, a C-grid, finite-volume method applied to Spherical Centroidal Voronoi Tessellations (SCVTs) where the mass, tracers, pressure and kinetic energy are defined at centers of the convex polygons and the normal component of velocity is located at cell edges. This method has many desirable mimetic properties, in spite of possessing low order of accuracy and inconsistencies that may constitute a potential problem for high resolution 3D models. In this work, we investigate a modification for the TRiSK scheme that will make it first order accurate in the maximum norm. Simulations compare the modified versus the original scheme for accuracy and stability.

Exponential Integrators for the Solution of the Tracer Equations in MPAS-Ocean
Sara Calandrini, post-doc, Phil Jones, Mark Petersen
Exponential time differencing (ETD) methods, also known as exponential integrators, constitute a class of numerical methods for the time integration of stiff systems of differential equations. Exponential integrators have recently gained attention in the ocean modeling community due to their stability properties that allow time steps considerably larger than those dictated by the CFL condition. We now have results obtained when such a scheme is applied within a full ocean circulation model.

Publication List

Publications

1. Capodaglio, G, Petersen, M.R., 2022. Local time stepping for the shallow water equations in MPAS-Ocean, J. Computational Physics 449, 110818, https://doi.org/10.1016/j.jcp.2021.110818.
2. Bishnu, S. (2021). Time-Stepping Methods for Partial Differential Equations and Ocean Models (Unpublished doctoral dissertation). Florida State University.
3. Bishnu, S., Petersen, M.P, Quaife, B. On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs. in review.
4. S. Calandrini, D. Engwirda, and M. Petersen. Comparing numerical accuracy and stability for different horizontal discretizations in MPAS-Ocean. Ocean Modelling, Volume 168, December 2021, 101908. https://doi.org/10.1016/j.ocemod.2021.101908
5. S. Calandrini, P.W. Jones, and M. Petersen. An exponential time differencing timestepping scheme for the tracer equations in MPAS-Ocean, 2021. in review.
6. Capodaglio, G, Petersen, M.R., Turner, A.K., Roberts, A.F. 2022. An unstructured C-grid type variational formulation for the sea ice dynamics, submitted to J. Computational Physics.
7. A Suite of Verification Exercises for the Barotropic Solver of Ocean Models. Siddhartha Bishnu, Mark Petersen, Bryan Quaife, in preparation for Journal of Advances in Modeling Earth Systems
8. Lilly, J., Capodaglio, G, Petersen, M.R., A coastal inundation test case for local time stepping in MPAS-Ocean, in preparation for Journal of Advances in Modeling Earth Systems

Presentations

1. Capodaglio, G. Local Time Stepping Schemes for Global to Coastal Simulations in MPAS-Ocean
   a. minisymposium talk at SIAM GS21 21, Online, June 21-24 2021.
   b. invited talk at the COSIM Webinar (Los Alamos National Lab), May 19 2021
   c. talk at the Los Alamos - Arizona Days 2021 Conference, Online, May 17-18 2021.
   d. invited minisymposium talk at SIAM CSE21, Online, March 1-5 2021.
2. Bishnu, S. COSIM Webinar Series (Virtual) Date: 02-23-2021
   Title: Time-Stepping Methods for PDEs and Ocean Models
3. Bishnu, S. Conference: SIAM Conference on Computational Science and Engineering 2021 i.e. CSE21 (Virtual) Date: 03-03-2021
   Title: A Suite of Verification Exercises for the Barotropic Solver of Ocean Models
4. Bishnu, S. Conference: Computational Xposition 2021, Department of Scientific Computing, Florida State University (Virtual) Date: 04-15-2021
   Title: On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs
5. Bishnu, S. Conference: SIAM Annual Meeting 2021 (Virtual) Date: 07-22-2021
   Title: On the Spatial and Temporal Order of Convergence of Hyperbolic and Parabolic PDEs
6. Bishnu, S. Minisymposium Organized Conference: SIAM Annual Meeting 2021 Dates: 07-22-2021 and 08-22-2021 Title: Novel Time-Stepping Methods with Applications in Computational Physics
7. Calandrini, S. An exponential time differencing time-stepping scheme for MPAS-Ocean - talk at the COSIM seminar at LANL, July 21, 2021.
8. Calandrini, S. A computational study on the TRiSK scheme instabilities in MPAS-Ocean - talk at the SIAM Conference on Mathematical & Computational Issues in Geoscience, Virtual Conference, June 22, 2021.
9. Calandrini, S. Exponential integrators for the solution of the tracer equations in MPAS-Ocean - talk at the SIAM Conference on Computational Science and Engineering, Virtual Conference, March 3 2021.

Financial Impact

The w20_ocean_time_step account supports the computational work of the following people and associated projects. All funding is under Office of Science, Office of Biological and Environmental Research (BER)

1. Mark Petersen: supported as part of the Energy Exascale Earth System Model (E3SM) project, and Integrated Coastal Modeling (ICOM)
2. Siddhartha Bishu: supported by the SciDAC projects LEAP (Launching an Exascale ACME Prototype) and CANGA (Coupling Approaches for Next Generation Architectures)
3. Giacomo Capodaglio: supported by Integrated Coastal Modeling ICOM
4. Sara Calandrini: supported by SciDAC project LEAP (Launching an Exascale ACME Prototype)
5. Nairita Pal: supported by Integrated Coastal Modeling ICOM
6. Jeremy Lilly: LANL student, supported by E3SM and SCGSR